

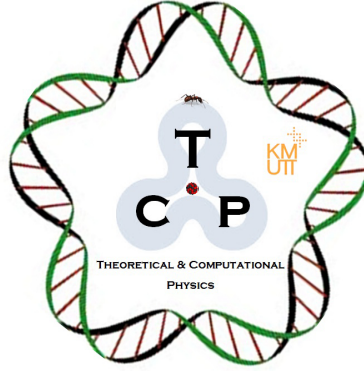
Theoretical model of charge mobility in DNA I: The path integral approach

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March 1, 2013



Abstract

A model of the charge-transfer process in DNA is investigated by using the Feynman path integral [14, 21, 49, 50]. The base-pairs' coordinates are eliminated resulting to the effective action of the system. The trial action is introduced in order to obtain the expectation value of the equation of motion. The electron will be in the equilibrium between lose and gain energy under the presence of an external electric field when the steady-state is reached. Using the result of the steady-state condition, the impedance function of the charge moving along the DNA chain is also studied. The mobility of charge moving in DNA was obtained and the limits at low and high temperature are also studied. The results of how the mobility depends on temperatures indicate that DNA may possibly be treated as a semiconductor quantum wire.

1 Introduction

DNA is one of the most important and complex structures of living organisms. In a nut shell, DNA is a nucleic acid containing the genetic instructions and plays a major role of the long-term storage of information, or a set of blueprints. The structure of DNA had been found to be the double helix, by Watson and Crick [53] at Cambridge University in 1953, composing of two polymers. These two polymers are glued together by base pairs which are the Adenin(A)-Thymine(T) and the Guanine(G)-Cytosine(C) pairs, see Fig. 1. Understanding all possible physical properties of DNA is one of the main quests of

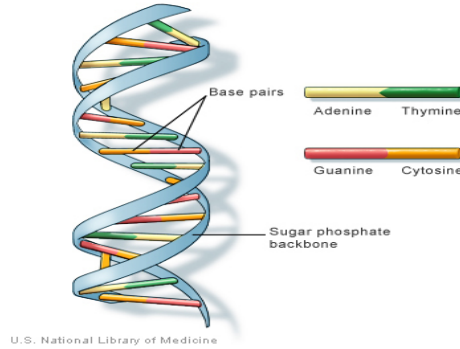


Figure 1: DNA is a double helix connected by the base-pairs, i.e., A-T and G-C [65].

Biophysicists. Studying the nature of charge transport mechanism in DNA molecule may gain more basic knowledge about signaling and repairing process of damaged DNA that are related to the mutation of the DNA resulting to cancer. The mechanism of charge transport through DNA could also be able to use to protect the damage, which is caused by oxidizing chemical [45, 20], of genomes in some organisms. Moreover, DNA could be possibly used as a tool to develop numerous tiny devices such as DNA biosensors, template for assembling nanocircuits and electric DNA sequencings, which are expected to be different from those existing traditional electronic devices [43, 44, 51, 52, 36].

There were many experimental results which indicate that DNA could be a conductor. The first confirmation was from Eley and Spivey [8] initiating that DNA exhibits conductor property. Consequently, scientists have been attracted to investigate the electronic properties of DNA. DNA could be a conductor because of the formation of a π -bond across the different A-T and C-G base-pairs. The π -stacking interaction is a key function for the electrical properties of other organic molecules. Fink et al., [11, 12] have shown the result of I-V characteristic of DNA suggesting that DNA is a conductor. Later, Porath et al., [43] have also been created an experiment to show that DNA could be treated as a large-band gap semiconductor. However, the charge transfer mechanisms in DNA chain are not yet well understood and remain very controversial¹. At temperature above 1 K, DNA may behave as conductors, semiconductors, insulator, while at below this temperature, DNA may exhibit a property as proximity-induced superconductor [42, 28, 11, 43, 61]. Interestingly in [61], the electric conductivity of λ -DNA using DNA covalently bonded to Au electrodes was investigated. They found that λ -DNA is an excellent insulator on the micron scale at room temperature.

Many theoretical models proposing to study the electrical properties of DNA were based on incoherent phonon-assisted hopping [32, 25], classical diffusion under the conditions of temperature-driven fluctuations [3], variable range hopping between localised states [57], transport via coherent tunneling [8] and polaron and soliton mechanisms [5, 33, 22, 23, 40, 56]. The quantum model of charge mobility has been studied by Lakhno [30, 31]. The Kohn theory was needed to approximated the model yielding that the mobility increases with the temperature decrease. Another approach is Feynman path integrals² which was used to study the ground-state energy and the effective mass of the electron in DNA by Natda [39]. In the present paper, we will concentrate on the theoretical description of the mobility of the charge moving

¹The literatures on DNA conductivity can be found in [19, 7, 9]

²The Feynman path integrals was successfully used to study the dynamic of the electron in the polar crystal [13, 14, 15, 50, 41, 21, 49, 58, 59, 60]

along a *model of one-dimensional DNA chain*. We use the path integral as a key technique to study the problem. The Hamiltonian of the system can be represented in the analogue form with Fröhlich's Hamiltonian suggesting that Feynman approach in polaron problem is applicable. We will show both analytical and numerical results of the study and we will try to give evidences: Could DNA be a conductor and what are the conditions and factors effecting to its conductivity. The structure of the paper is organised in the following. In section 2, we will discuss the model of one-dimensional DNA. The path integral method is used to eliminated the coordinates of the harmonic chains in DNA leading to the effective action of the system. In section 3, the steady-state condition at finite temperatures of the charge in DNA chain under the presence of the external electric field is studied. In section 4, the impedance function is computed from the equation of motion by relaxing the steady-state condition. Furthermore, the mobility at low temperatures of the charge is studied with varying the coupling constants and number of base-pairs. The effective mass at zero temperature of the charge interacting with DNA chain are also calculated. In section 5, the physical concept of the analytical analysis and numerical results in the previous sections will be presented. In section 6, the summary of results and some open problems along with possible future developments will be mentioned.

2 The model of charge transport in one dimensional DNA chain

DNA composes of two major long polymers which are made from repeating units called nucleotides. For all living things, DNA is in the shape of a double helix which is bonded together with backbones made from alternating phosphate and sugar residues, i.e., A-T and C-G pairs. As mentioned that DNA has a double helix structure which is complicated form. Then in this paper, the structure of DNA will be simplified by stretching a DNA chain into one dimension as shown in Fig. 2. The aim of the current study is to show the effect of the length, coupling constant and temperatures to the charge mobility in DNA. The electron is now moving along the DNA chain with N base-pairs and there is the interaction

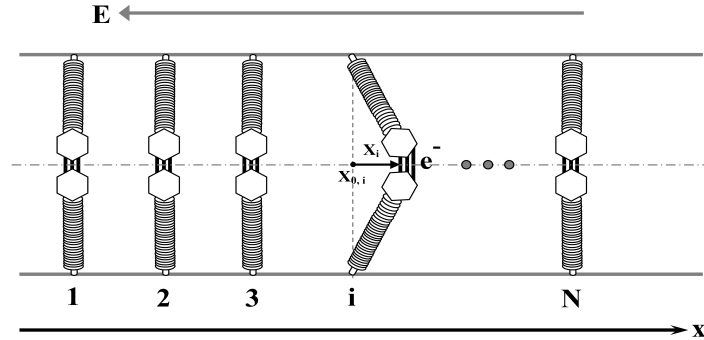


Figure 2: A model of one-dimensional DNA chain. The base-pairs, which will be treated to have the same physical structure, are represented by oscillators which will move back and forth along the x -direction.

between the electron and base-pairs throughout the chain. The Hamiltonian of the model proposed by Natda [39] is given by

$$H_{e-DNA} = \frac{p^2}{2m} + \frac{1}{2} \sum_{i=1}^N \left[\frac{P_i^2}{M} + M\Omega^2 x_i^2 \right] + M\Omega^2 \alpha \sum_{i=1}^N x_i \delta(x - x_{0,i}). \quad (2.1)$$

The first term is the kinetic energy where p and m are the momentum and mass of the charge, respectively. The second term represents the harmonic oscillators of the i th base-pair(backbone) where M and Ω are the mass and oscillation frequency for each base-pair and x_i is the displacement along the x -axis of the i th from its equilibrium $x_{0,i}$. The last term describes the interaction³, which is modeled by Dirac delta function, between electron and the base-pairs where α is the coupling constant.

³We assume that the interaction will take place only on the i th base-pair(distorted), not for other base-pairs(undistorted).

The action of the system is now

$$S_{e-DNA} = \int_0^T dt \left(\frac{m\dot{x}^2}{2} + \frac{M}{2} \sum_{i=1}^N \left[\frac{\dot{x}_i^2}{M} - \Omega^2 x_i^2 \right] - M\Omega^2 \alpha \sum_{i=1}^N x_i \delta(x - x_{0,i}) \right), \quad (2.2)$$

and the propagator can be written in the form

$$I_{e-DNA} = \int_{x(0)}^{x(T)} \mathcal{D}[x(t)] \prod_{i=1}^N \int_{x_i(0)}^{x_i(T)} \mathcal{D}[x_i(t)] e^{\frac{i}{\hbar} S_{e-DNA}}. \quad (2.3)$$

Using Feynman path integral method [13, 49, 15, 39], the base-pairs' coordinates can be eliminated resulting to the effective propagator

$$I_{eff} = \int_{x(0)}^{x(T)} \mathcal{D}[x(t)] e^{\frac{i}{\hbar} S_{eff}}, \quad (2.4)$$

where the S_{eff} is the effective action given by

$$S_{eff} = \int_0^T dt \left(\frac{m\dot{x}^2}{2} + \frac{M\Omega^3 \alpha^2}{4} \sum_{i=1}^N \int_0^T d\sigma f_i(t, \sigma) \frac{\cos(\Omega|t - \sigma| - T/2)}{\sin(\Omega T/2)} \right), \quad (2.5)$$

where $f_i(t, \sigma) = \delta[x(t) - x_{0,i}] \delta[x(\sigma) - x_{0,i}]$. Using the fact that $\sum_i \delta[x(t) - x_{0,i}] \delta[x(\sigma) - x_{0,i}] = N \delta[x(t) - x(\sigma)]$, the effective action becomes

$$S_{eff} = \int_0^T dt \left(\frac{m\dot{x}^2}{2} + \eta \int_0^T d\sigma \int_{-\infty}^{\infty} dk e^{ik(x(t) - x(\sigma))} \frac{\cos(\Omega|t - \sigma| - T/2)}{\sin(\Omega T/2)} \right), \quad (2.6)$$

since $\delta[x(t) - x(\sigma)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x(t) - x(\sigma))}$ and we define $\eta \equiv \frac{M\Omega^3 \alpha^2 N}{8\pi}$. After eliminating the base-pairs' coordinate, the action of the system (2.6) can be written as a function of the electron coordinate.

3 The steady-state condition

In this section, we consider the system of the electron moving along the DNA chain under the influence of the external constant electric field E_0 . The Hamiltonian of the system now is

$$H_{e-DNA} = \frac{p^2}{2m} - E_0 x + \frac{1}{2} \sum_{i=1}^N \left[\frac{P_i^2}{M} + M\Omega^2 x_i^2 \right] + M\Omega^2 \alpha \sum_{i=1}^N x_i \delta(x - x_{0,i}). \quad (3.1)$$

When the electric field is turn on, the electron will be accelerated. However, electron will interact with the base-pairs while it moves along the DNA chain resulting to loose some amount of energy to base-pairs. Then if we leave the system long enough the system will reach the steady-state.

In order to get the steady-state condition, we will apply the method, called Double path integral [14, 49, 50, 60], that was used to study the motion of the electron in the polar crystal. Let ρ be the density matrix of the system and the expectation value of any operator \mathbf{Q} at time t given by

$$\langle \mathbf{Q}(t) \rangle = \text{Tr}(\mathbf{Q}\rho(t)). \quad (3.2)$$

We now assume that the system is in the thermal equilibrium initially, $\rho(t=0) = \exp(-\beta H_{e-DNA})$ where $\beta = 1/k_B T$, T and k_B are the temperature and Boltzmann constant, respectively. To obtain the density matrix at any time t , we need to solve the time-evolution equation

$$i\hbar \frac{\partial \rho}{\partial t} = [H_{e-DNA}, \rho], \quad (3.3)$$

and therefore we have⁴

$$\rho(t) = e^{-\frac{i}{\hbar} \int_0^T H(s) ds} \rho(0) e^{+\frac{i}{\hbar} \int_0^T H'(s) ds} . \quad (3.4)$$

As we mentioned earlier that at the beginning the DNA is in thermal equilibrium, then we may write $\rho(0) = \exp(-\beta \sum_k a_k^\dagger a_k)$ where a_k^\dagger and a_k are creation and annihilation operators of the base-pairs.

Next, we will compute the expectation value of electron's displacement at time T

$$\langle x(T) \rangle = \frac{\partial}{\partial \gamma} \text{Tr} \rho(T) |_{\gamma=0} , \quad (3.5)$$

where we now put $E_0 \rightarrow E_0 + \gamma \delta(t-T)$ and $E'_0 \rightarrow E'_0$. The problem of integrating $\text{Tr} \rho(T)$ over DNA base-pairs' coordinate can be performed in the same fashion as we mentioned in section 2. For the convenient, we transform the electron coordinate to a frame of reference drifting [49, 14, 50] with the expectation value of the electron's velocity v : $x(t) = y(t) + vt$. Then $\text{Tr} \rho(T)$ can be written in the form

$$\text{Tr} \rho(T) = \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] e^{i\Psi_e} , \quad (3.6)$$

where

$$\Psi_e = \Phi_e + \Phi'_e + \Phi_{in} , \quad (3.7a)$$

$$\Phi_e = \int_0^T \left(\frac{m}{2} \dot{y}^2(t) + (E_0 + \gamma \delta(t-T)) y(t) \right) , \quad (3.7b)$$

$$\Phi'_e = \int_0^T \left(\frac{m}{2} \dot{y}'^2(t) + E'_0 y'(t) \right) , \quad (3.7c)$$

$$\begin{aligned} \Phi_{in} = & i\eta \int_{-\infty}^{\infty} dk \int_0^T dt \int_0^T d\sigma \left(S_{\Omega}(t-\sigma) e^{-ik(y'(t)-y'(\sigma))} + S_{\Omega}^*(t-\sigma) e^{ik(y(t)-y(\sigma))} \right. \\ & \left. - S_{\Omega}(t-\sigma) e^{ik(y'(t)-y(\sigma))} - S_{\Omega}^*(t-\sigma) e^{ik(y(t)-y'(\sigma))} \right) , \end{aligned} \quad (3.7d)$$

$$S_{\Omega}(u) = \left(\frac{e^{i\Omega u}}{1 - e^{-\beta\Omega}} + \frac{e^{-i\Omega u}}{e^{\beta\Omega} - 1} \right) e^{-ikv t} . \quad (3.7e)$$

Here comes to the crucial point. The path integral of (3.6) could not be performed exactly, then we need to introduce a trail action given by

$$\Psi_{tr} = \Phi_e + \Phi'_e + \Phi_{tr} , \quad (3.8)$$

where

$$\begin{aligned} \Phi_{tr} = & i \int_{-\infty}^{\infty} dk \int_0^T dt \int_0^T d\sigma \left(G(t-\sigma) (y'(t) - y'(\sigma))^2 + G^*(t-\sigma) (y(t) - y(\sigma))^2 \right. \\ & \left. - G(t-\sigma) (y'(t) - y(\sigma))^2 - G^*(t-\sigma) (y(t) - y'(\sigma))^2 \right) , \end{aligned} \quad (3.9a)$$

$$G(u) = \sum_{j=1}^N \int_{-\infty}^{\infty} d\Omega'_j G(\Omega'_j) e^{-i\Omega'_j u} . \quad (3.9b)$$

The function $G(\Omega'_j)$ is the distribution function⁵ [14, 49] with frequencies $\Omega'_j = \sqrt{\frac{K_j}{M'}}$ of j th fictitious particle as shown in Fig. 3. We now expand (3.6) in the form

⁴An unprimed operator acts to the left and ordered right to left with increasing time, and primed operator acts to the right and ordered left to right with increasing time.

⁵In reference [13, 14, 49, 50, 39], they considered only one fictitious particle. The reason why we consider N' fictitious particles is to make trial action more realistic and also to improve the variational result [1, 2].

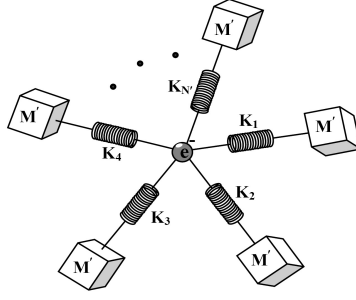


Figure 3: The electron is attached to N' fictitious particles of mass M' with different coupling constant K_j corresponding to each one of them.

$$\begin{aligned}
\int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] e^{i\Psi_e} &= \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] e^{i\Psi_{tr}} e^{i(\Psi_e - \Psi_{tr})} , \\
&= \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] e^{i\Psi_{tr}} (1 + i(\Psi_e - \Psi_{tr}) + \dots) . \quad (3.10)
\end{aligned}$$

Using (3.10), we possibly write

$$\langle y(T) \rangle_e = \langle y(T) \rangle_{tr} + {}_e \langle y(T) \rangle_{tr} - {}_{tr} \langle y(T) \rangle_{tr} + \dots , \quad (3.11)$$

where

$${}_j \langle y(T) \rangle_k = \frac{\partial}{\partial \gamma} \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] i\Psi_j e^{i\Psi_k} |_{\gamma=0} , \quad (3.12a)$$

$$\langle y(T) \rangle_k = \frac{\partial}{\partial \gamma} \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] e^{i\Psi_k} |_{\gamma=0} . \quad (3.12b)$$

The velocity of the electron can also be expanded in the form

$$v_e = v_{tr} + {}_e v_{tr} - {}_{tr} v_{tr} + \dots , \quad (3.13)$$

We are interested to calculate the expectation value of the velocity at $T \rightarrow \infty$ which the steady-state is reached. Then we have

$${}_j v_k = \lim_{T \rightarrow \infty} \frac{d}{dT} {}_j \langle y(T) \rangle_k , \quad (3.14a)$$

$$v_k = \lim_{T \rightarrow \infty} \frac{d}{dT} \langle y(T) \rangle_k . \quad (3.14b)$$

From the relation (3.13), we may find

$$\frac{1}{v_e} = \frac{1}{v_{tr}} - \frac{{}_e v_{tr} - {}_{tr} v_{tr}}{v_{tr}^2} , \quad (3.15)$$

which is nothing more than the first order expansion of the reciprocal of $v_e \simeq v_{tr} + {}_e v_{tr} - {}_{tr} v_{tr}$. The reason why we choose such an expansion for this type of problem is given in reference [14, 49, 50]. Moreover, assuming $v_{tr} = - {}_{tr} v_{tr}$ which reduces (3.15) to

$$\frac{1}{v_e} = - \frac{{}_e v_{tr}}{v_{tr}^2} . \quad (3.16)$$

From (3.12b), we find that

$$\langle y(T) \rangle_e = -iE_0 \int_0^T dt (L(t) - L^*(t)) , \quad (3.17)$$

where

$$L(t) - L^*(t) = \int_{-\infty}^{\infty} \frac{d\nu}{2\pi i} \left(\frac{1}{Z_\nu} - \frac{1}{Z_\nu^\dagger} \right) e^{-i\nu t}, \quad (3.18a)$$

$$Z_\nu = -\nu^2 - 4\nu \sum_{j=1}^{N'} \int_{-\infty}^{\infty} \frac{d\Omega'_j}{\Omega'_j} \frac{G(\Omega'_j)}{\Omega_j'^2 - \nu^2}. \quad (3.18b)$$

The first order of velocity in the expansion is

$$v_{tr} = -i2E_0 \text{Im}L(T). \quad (3.19)$$

The next velocity in the expansion v_{tr} can be computed by considering the term $\int \int \Psi_e e^{\Psi_{tr}}$

$$\begin{aligned} \int \mathcal{D}[y(t)] \int \mathcal{D}[y'(t)] i\Psi_e e^{i\Psi_{tr}} &= -\eta \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\theta \int_{-\infty}^{\theta} d\zeta \left(S_\Omega(\theta - \zeta) \int \int (1) \right. \\ &\quad \left. + S_\Omega^*(\theta - \zeta) \int \int (2) - S_\Omega(\theta - \zeta) \int \int (3) - S_\Omega^*(\theta - \zeta) \int \int (4) \right). \end{aligned} \quad (3.20)$$

We introduce the shorthand notations where the force terms $\int \int [E_0, E'_0]$ in $\int \int \Psi_e e^{\Psi_{tr}}$ will be inserted as follows

$$\int \int (1) = \int \int [E_0 + \gamma\delta(t - T), E'_0 + k(\delta(t - \theta) - \delta(t - \zeta))], \quad (3.21a)$$

$$\int \int (2) = \int \int [E_0 + \gamma\delta(t - T) + k(\delta(t - \theta) - \delta(t - \zeta)), E'_0], \quad (3.21b)$$

$$\int \int (3) = \int \int [E_0 + \gamma\delta(t - T) + k\delta(t - \theta), E'_0 + k\delta(t - \zeta)], \quad (3.21c)$$

$$\int \int (4) = \int \int [E_0 + \gamma\delta(t - T) + k\delta(t - \zeta), E'_0 + k\delta(t - \theta)]. \quad (3.21d)$$

After performing a tedious computation, we put v_{tr} into (3.16) together with another assumption that $v_e \simeq v_{tr} \equiv v$ yielding the steady-state equation

$$E_0 = \eta \int_{-\infty}^{\infty} d\zeta \int_{-\infty}^{\infty} dk \frac{k \cos[\Omega\zeta]}{\sinh[\Omega\beta/2]} e^{-ikv(\zeta + i\beta/2)} e^{-k^2 \Delta_\beta(\zeta)}, \quad (3.22)$$

where

$$\Delta_\beta(u) = \frac{1}{2} \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'} (z_j^2 - \Omega_l'^2)}{z_j \prod_{m \neq j} (z_j - z_m)} \frac{\cosh[z_j\beta/2] - \cos[z_j u]}{\sinh[z_j\beta/2]}, \quad (3.23)$$

and z_j are the roots of the polynomial

$$\nu^2 \prod_{j=1}^{N'} (\nu^2 - \Omega_j'^2) - \nu^2 \sum_{j=1}^{N'} \Omega_j'^2 = 0. \quad (3.24)$$

(3.22) represents the equation of motion in the steady-state condition, which holds at any temperatures, for the charge moving along the DNA chain according to the model (2.1). The charge gains the energy from the electric field and gives the energy to the base-pairs via the interaction. Note that we compute the velocity only the first order in the expansion (3.13) corresponding to the fact that the interaction between the electron and base-pairs is weak. The expansion in (3.11) can be pushed further in order to cover the higher range of the interaction.

4 Electrical properties of the DNA

In the previous section, the steady-state equation is obtained by looking the expansion of the velocity of the electron moving along DNA chain. For the present section, we will compute the impedance function

of the system from the equation of motion. The electric field is now modified to $E_0 \rightarrow E(t) = E_0 e^{i\varpi t}$ where ϖ is the oscillation frequency. From (3.17), we may write

$$\langle y(T) \rangle_e = -i \int_0^T dt Y(T-t) E(t). \quad (4.1)$$

Taking the Fourier transform of (4.1), we have

$$y_\varpi = Y_\varpi E_\varpi, \quad (4.2)$$

where Y_ϖ is the Fourier transform of the response function given by

$$Y_\varpi = \int_0^T d\xi e^{i\varpi\xi} \int_0^T \frac{d\nu}{2\pi i} \left[\frac{1}{Z_\nu} - \frac{1}{Z_\nu^\dagger} \right] e^{-i\nu\xi} \equiv \frac{1}{Z_\varpi}. \quad (4.3)$$

The Z_ϖ is the impedance function of the electron moving on DNA chain. Without imposing the steady-state condition, the equation of motion reads

$$E(T) = \eta \int_{-\infty}^{\infty} d\zeta \int_{-\infty}^{\infty} dk \frac{k \cos[\Omega\zeta]}{\sinh[\Omega\beta/2]} e^{-ikv(\zeta+i\beta/2)} e^{-k^2\Delta_\beta(\zeta)} + \langle \ddot{y}(T) \rangle_e. \quad (4.4)$$

Applying (4.1) to (4.4), we find that the impedance function can be expressed in the form

$$Z_\varpi = -\varpi^2 + \int_0^\infty d\xi (1 - e^{i\xi\varpi}) \text{Im} S(\xi), \quad (4.5)$$

where

$$S(\xi) = 2\eta \int_{-\infty}^{\infty} dk k^2 \left(\frac{e^{i\Omega\xi}}{1 - e^{-\beta\Omega}} + \frac{e^{-i\Omega\xi}}{e^{\beta\Omega} - 1} \right) e^{-k^2\Lambda_\beta(\xi)}, \quad (4.6a)$$

$$\Lambda_\beta(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'} (z_j^2 - \Omega_l'^2)}{z_j \prod_{m \neq j} (z_j - z_m)} \frac{\cosh[z_j\beta/2] - \cos[z_j(u - i\beta/2)]}{\sinh[z_j\beta/2]}. \quad (4.6b)$$

We are now interested for the case of $\varpi < 1$ and $\beta \rightarrow \infty$ (zero temperature) and the path of integration along the real axis may be rotated to a path along the positive or negative imaginary axis $\xi \simeq 0$ to $\pm i\infty$ [14]. The impedance becomes

$$Z_\varpi = -\varpi^2 - 2\eta \int_0^\infty d\xi (1 - \cosh[\varpi\xi]) e^{-\Omega\xi} \int_{-\infty}^{\infty} dk k^2 e^{-k^2\Lambda(\xi)}, \quad (4.7)$$

where

$$\Lambda(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'} (z_j^2 - \Omega_l'^2)}{z_j \prod_{m \neq j} (z_j - z_m)} (1 - e^{-z_j u}). \quad (4.8)$$

In the case of extremely low frequency ϖ , we may approximate $1 - \cosh[\varpi\xi] \cong -\varpi^2 \xi^2/2$. Then the impedance function is simplified to

$$Z_\varpi = -\varpi^2 m^*, \quad (4.9)$$

where m^* is the effective mass given by

$$m^* = 1 + \frac{\eta\sqrt{\pi}}{2} \int_0^\infty d\xi \xi^2 \frac{e^{-\Omega\xi}}{[\Lambda(\xi)]^{3/2}}. \quad (4.10)$$

(4.9) together with (4.10) suggest that the charge behaves like a free particle with the effective mass m^* when it moves along the DNA chain. According to the model, (4.7) is the impedance function for the whole DNA chain which consists of N base-pairs. If we assume that for each base-pair has the same impedance, we find

$$z_\varpi = \frac{Z_\varpi}{N}, \quad (4.11)$$

which is the impedance for each base-pair. Then the system can be presented as the connected series of the impedance function shown in Fig.4. In the case that N becomes very large $N \rightarrow \infty$ the impedance function remains finite

$$\lim_{N \rightarrow \infty} z_{\varpi} = -2\eta' \int_0^{\infty} d\xi (1 - \cosh[\varpi\xi]) e^{-\Omega\xi} \int_{-\infty}^{\infty} dk k^2 e^{-k^2 \Lambda(\xi)}, \quad (4.12)$$

where $\eta' = \frac{M\Omega^3\alpha^2}{8\pi}$. From the result (4.11), we see that the conductivity of the DNA is directly proportional to the reciprocal of the length of DNA [63].

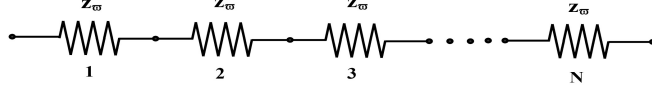


Figure 4: DNA chain can be represented as the connected series of the impedance function z_{ϖ} .

We now introduce the function

$$\chi_{\varpi} = \int_0^{\infty} d\xi (1 - e^{i\xi\varpi}) \text{Im}S(\xi), \quad (4.13)$$

which is the last term of the impedance function (4.5). For the convenient for analytical analysis as mentioned in [14, 49, 50], we may consider

$$\text{Im}\chi_{\varpi} = \sinh[\varpi\beta/2] \int_0^{\infty} du \cos[\varpi u] \Sigma(u), \quad (4.14)$$

where

$$\Sigma(u) = S(u + i\beta/2) = \frac{2\eta}{\sqrt{\pi}} \frac{\cos[u]}{\sinh[\beta/2]} \frac{1}{[D_{\beta}(u)]^{3/2}}, \quad (4.15a)$$

$$D_{\beta}(u) = \sum_{j=1}^{2N'+1} \frac{\prod_{l=1}^{N'} (z_j^2 - \Omega_l'^2)}{z_j \prod_{m \neq j} (z_j - z_m)} \frac{\cosh[z_j\beta/2] - \cos[z_j u]}{\sinh[z_j\beta/2]}. \quad (4.15b)$$

The mobility [14, 49, 50] of the charge moving along DNA chain is defined

$$\frac{1}{\mu} = \lim_{\varpi \rightarrow 0} \frac{\text{Im}\chi_{\varpi}}{\varpi} = \frac{\beta}{2} \int_0^{\infty} \Sigma(u) du. \quad (4.16)$$

We see that the mobility of the charge is a function of the temperature and also the coupling constant α . We also would like to point that (4.14) and (4.16) hold at any temperatures. In the next section, we will show the analytical analysis as well as the numerical results of the effective mass and the charge mobility.

5 Physical concept of the results

In this section, we will focus more the physical meaning of the results from the previous sections. Before proceeding, we need to reduce the complexity of the trial action (3.8). Here, we are interested in the case of $N' = 1$. Let v and Ω' be the variational variables, determined from the minimization of the ground state energy [39, 13], given by

$$\Omega' = \sqrt{\frac{K}{M'}}, \quad \text{and} \quad v = \sqrt{\frac{K}{\varrho}}, \quad \text{and} \quad \varrho = \frac{m}{m + M'}. \quad (5.1)$$

The steady-state condition: With $N' = 1$, the (3.22) becomes

$$E_0 = \eta \int_{-\infty}^{\infty} d\zeta \int_{-\infty}^{\infty} dk k \left([1 + n(\Omega)] e^{i(\Omega - kv)\zeta} - n(\Omega) e^{-i(\Omega - kv)\zeta} \right) e^{-k^2 D_{\beta}(\zeta)}, \quad (5.2)$$

where

$$n(\Omega) = \frac{1}{e^{\beta\Omega} - 1}, \quad (5.3a)$$

$$D_\beta(u) = \frac{1}{2} \frac{\Omega'^2}{v^2} \left[\left(\frac{v^2 - \Omega'^2}{v\Omega'^2} \right) \frac{\cosh[v\beta/2] - \cos[v(u - i\beta/2)]}{\sinh[v\beta/2]} - iu + \frac{u^2}{\beta} \right]. \quad (5.3b)$$

We will follow the analysis process of (5.2) as those in [49, 41]. We start to rewrite (5.3b) in the following form [41]

$$D_\beta(u) = \frac{1}{2} \left(\frac{v^2 - \Omega'^2}{v^3} \right) \coth[v\beta/2] - \frac{iu}{2M} + \frac{u^2}{2M\beta} - \left(\frac{v^2 - \Omega'^2}{v^3} \right) ([1 + n(v)]e^{-iviu} + n(v)e^{ivu}), \quad (5.4)$$

where $M = \frac{\Omega'^2}{v^2}$. We now also introduce the relation [49, 41]

$$e^{-\frac{k^2 u^2}{2M\beta}} = \int dp f(p) e^{\pm \frac{ipku}{M}}, \quad \text{where} \quad f(p) = \sqrt{\frac{\beta}{2\pi M}} e^{-\frac{\beta p^2}{2M}}. \quad (5.5)$$

Inserting (5.5) and (5.4) into (5.2) together with expanding the terms $[1 - n(v)]$ and $n(v)$ in the Taylor series, we obtain

$$\begin{aligned} E_0 = & \eta \sqrt{\frac{\beta}{2\pi}} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int dp \int_{-\infty}^{\infty} dk B(\beta, n, n') k^{2(n+n'-1)} e^{-\frac{k^2}{2} \left(\frac{v^2 - \Omega'^2}{v^3} \right) \coth[v\beta/2]} f(p) k \\ & \times \left\{ [1 + n(\Omega)] \cdot \delta \left(\Omega - k \left(v + \frac{p}{M} \right) + \frac{k^2}{2M} + (n - n')v \right) \right. \\ & \left. - n(\Omega) \cdot \delta \left(-\Omega + k \left(v + \frac{p}{M} \right) + \frac{k^2}{2M} + (n - n')v \right) \right\}, \quad (5.6) \end{aligned}$$

where

$$B(\beta, n, n') = \frac{\frac{1}{2} \left[\left(\frac{v^2 - \Omega'^2}{v^3} \right) [1 + n(v)] \right]^n}{n!} \frac{\frac{1}{2} \left[\left(\frac{v^2 - \Omega'^2}{v^3} \right) n(v) \right]^{n'}}{n'!}. \quad (5.7)$$

The physical meaning of (5.6) is the following, see also [49, 41]. The term in the second line of (5.6), with the term $[1 + n(\Omega)]$, represents the process that the electron with momentum $p + Mv$ emits a phonon with energy Ω and momentum k , while the electron state changes from $n' \rightarrow n$ as shown in Fig.5(a). The electron momentum is reduced by k and the delta function tells that energy is conserved, while the $[1 + n(\Omega)]$ shows the a phonon with frequency Ω is emitted. The term in the third line of (5.6), with the term $n(\Omega)$, describes the opposite situation as follows: the electron with momentum $p + Mv$ absorbs the phonon frequency Ω as shown in Fig.5(b).

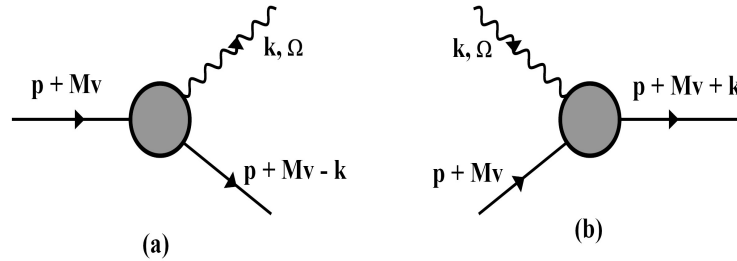


Figure 5: The scattering processes of the electron (a solid line) by phonon (a wavy line). (a) a electron with momentum $p + Mv$ in n' state emits a phonon with momentum k and energy Ω . The electron changes to a new state n with momentum $p + Mv - k$. (b) shows the opposite situation in which the phonon is absorbed.

The effective mass: The effective mass (4.10) can be simplified onto the form

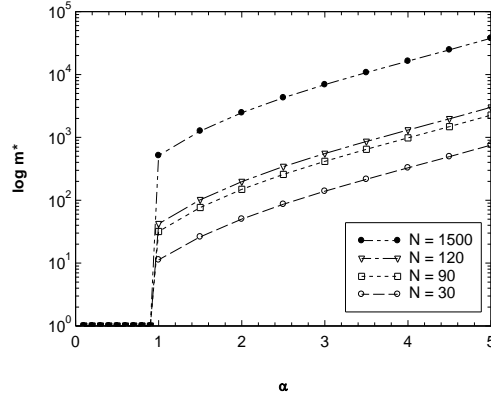


Figure 6: Coupling interaction dependence of the effective mass for different number of base-pairs. The dashed, dotted, dot-dashed and two-dot-dashed lines are dependence of the effective mass when the number of base pairs are $N = 30, 90, 120$ and 1500 , respectively.

$$m^* = 1 + \eta\sqrt{8\pi}v^3 \int_0^\infty d\xi \frac{\xi^2 e^{-\Omega\xi}}{[v(1 - \frac{\Omega'^2}{v^2})(1 - e^{-v\xi}) + \Omega'^2\xi]^{3/2}}. \quad (5.8)$$

which agrees with [39] (with replacement ρ with N). The numerical results of the effective mass with various coupling constants and the number of base-pairs are shown in Fig. 6. In the case of the weak coupling, the electron will move freely as the effective mass becomes the mass of the electron: $m^* \rightarrow m = 1$. In the case of the strong coupling, the electron will behave like a heavy particle as the effective mass increases. In the case of damaged DNA, the coupling constant of the base-pairs may possibly change to be in the strong coupling regime or another way around, then there is a potential to use the effective mass of the electron to detect the damage in DNA. Another effect to the mass of the electron is the number of the base-pairs N . For the large number N , the effective mass of the electron will increase drastically. This result suggests that the length of the DNA has effect to the charge transfer mechanism as pointed in [63].

The mobility: We consider the function $\text{Im}\chi_\varpi$ for the case $N' = 1$

$$\text{Im}\chi_\varpi = \frac{4\sqrt{2}\eta\beta^{3/2}}{\sqrt{\pi}} \left(\frac{v}{\Omega'}\right)^3 \frac{\sinh[\varpi\beta/2]}{\sinh[\beta/2]} \int_0^\infty \frac{\cos[\varpi u] \cos[u] du}{\left[u^2 + \frac{\beta^2}{4} + \beta \left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right) \coth[\beta v/2] - \beta \left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right) \frac{\cos[vu]}{\sinh[\beta v/2]}\right]^{3/2}}. \quad (5.9)$$

We see that the integrand of (5.9) has the same structure with those (47a) in [14]. If we now consider the system at low temperatures and $\varpi < 1$ we have

$$\begin{aligned} \text{Im}\chi_\varpi = & 4\sqrt{2}\eta \left(\frac{v}{\Omega'}\right)^3 \left[\sqrt{1 - \varpi} e^{-\beta(1-\varpi)} e^{-\left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right)(1-\varpi)} + \sqrt{1 + \varpi} e^{-\beta} e^{-\left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right)(1+\varpi)} \right. \\ & \left. - \sqrt{1 - \varpi} e^{-\beta} e^{-\left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right)(1-\varpi)} - \sqrt{1 + \varpi} e^{-\beta(1+\varpi)} e^{-\left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right)(1+\varpi)} \right]. \end{aligned} \quad (5.10)$$

The first term describes the process that the electron absorbs a quantum energy ϖ from the electric field and emits a phonon with unit energy. The second term shows that the electron absorbs a quantum energy ϖ and also absorbs a phonon then at the end the electron will carry the momentum $\sqrt{1 + \varpi}$. The third term, the electron absorbs a phonon and releases a quantum energy ϖ to the electric field. The fourth term represents the electron with energy $1 + \varpi$ emitting a phonon as well as a quantum energy to the electric field. The term $\exp[-\left(\frac{v^2 - \Omega'^2}{\Omega'^2 v}\right)(1 \pm \varpi)]$ tells the chance that the electron with energy $1 \pm \varpi$ completes the processes. Eq(5.10) contains possible scatterings happening while the electron moving along the DNA chain as shown in Fig. 7.

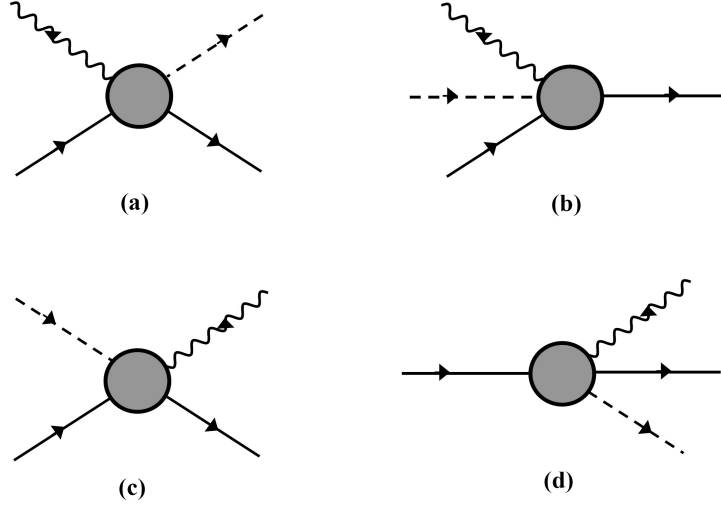


Figure 7: The scattering processes of the electron (a solid line) absorbing and emitting a quantum energy (a wavy line) and a phonon (a dashed line).

In the case of low temperatures and $\varpi \rightarrow 0$, (5.9) leads to the dc mobility

$$\frac{1}{\mu} = 4\eta\sqrt{\frac{2}{\pi}}\beta^{3/2}\left(\frac{v}{\Omega'}\right)^3 \int_0^\infty \frac{\cos[u]du}{\left[2\left(\frac{v^2-\Omega'^2}{\Omega'^2}\right)\frac{1-\cos[vu]}{v^2} + u^2 + \frac{\beta^2}{4}\right]^{3/2}}. \quad (5.11)$$

As we explained (5.10) that the electron may be scattered by oscillations of the base-pairs (phonons) which will be increased with the temperature. We are interested for the case of weak coupling because some future analysis can be done on the mobility (5.11). In this case, the variational variables $\Omega' \approx v$ leading to

$$\frac{1}{\mu} = 4\eta\sqrt{\frac{2}{\pi}}\beta^{3/2} \int_0^\infty \frac{\cos[u]du}{\left[u^2 + \frac{\beta^2}{4}\right]^{3/2}} = 2\eta\sqrt{\frac{2}{\pi}}\beta^{1/2}K_1(\beta);, \quad (5.12)$$

where K_1 is the modified Bessel function of second kind.

At high temperatures, $\beta \rightarrow 0$ and $K_1(\beta) \approx 1/\beta$, the mobility becomes

$$\frac{1}{\mu} \propto \frac{1}{\sqrt{\beta}} \Rightarrow \mu \propto T^{-1/2}. \quad (5.13)$$

At high temperatures, electron-optical phonon interaction will play an important role in quantum wires of non-polar semiconductors which the mobility is affected strongly by the optical phonon scattering so the mobility is expected to be proportional to $T^{-1/2}$ [64, 10]. For our result in (5.13), we observed that at high temperatures the behavior of the mobility in the case of DNA chain is similar to that in the semiconductors quantum wires expression. We found $\mu \propto T^{-1/2}$, indicating that optical phonon scattering dominates the temperature dependence of the DNA mobility for weak coupling.

At low temperatures, $\beta \rightarrow \infty$ and $K_1(\beta) \approx e^\beta/\sqrt{\beta}$, the mobility becomes

$$\mu \propto e^\beta. \quad (5.14)$$

The electron mobility will be influenced strongly by the interaction of the electrons with phonons. In a semiconductor quantum wire, the mobility of an electron interacting with acoustic phonons would follow an exponential behavior and the energy relaxation of an electron due to emissions of acoustic phonon strongly increased by all low temperatures acoustic phonon scattering mechanisms, which are exponentially activated in an electron [62, 4]. In weak coupling systems of DNA chain, the low-temperature behavior of its

mobility has the characteristic form of an exponential term. The feature of our results is the identification of electron transfer in the DNA similar to be behavior of electron scattering in a semiconductor quantum wire. Recent studies of the electrical conductivity of DNA molecules reveal that they may act as semiconductor materials with nanometer scale dimensions [6, 48, 34, 35, 26, 27, 56, 29, 38, 43, 11, 28, 24, 17, 7].

6 Summary

We study the model of charge transfer in one-dimensional DNA chain with arbitrary N base-pairs. The base-pairs have been modeled as the oscillators and the interaction between the charge and the oscillator is represented by the Dirac delta function. The path integral method is used as the key tool to study the physical properties of the system. The main advantage of path integral is that the base-pairs' coordinates can be integrated over leading to the effective action. The expectation value of the equation of motion of the electron moving in DNA chain under the influence of the external electric field can be computed by introducing the trial action. The electron will gain energy from the electric field and will give some to the phonons via the scattering process. In steady-state condition, the electron is the balance of these two processes. The electron will behave like a heavy particle if the coupling constant and the number of base-pairs are large. On the other hand, the electron will move freely in weak coupling region and small number of base-pairs.

In the present paper, the mobility of charge moving along DNA chain is studied as a major feature. The study of mobility both at low and high temperatures suggests that DNA can be possibly treated as a semiconductor quantum wire. For the case of extremely low temperatures, the mobility is very high reflecting a very high conductivity. This result may be possibly explained by the resonant tunneling effect. According to our knowledge, the mobility of charge along DNA has not yet been measured directly and most of the experiments were focused at room temperature or high temperatures [9]. Then there is a difficulty to compare our results with the experiments, just some of them as we did explain in the main text before.

The hopping process [46, 16] may be a current candidate to theoretically explain the charge transfer in DNA and indeed there are many experimental results supported [47, 55, 18]. However, experiments have so many factors as well as conditions that need to be controlled leading to a wide range of the results. This causes a big debate on what should DNA conductivity be as pointed out in [9, 7]. Then, we believe that the model in this paper may offer an alternative theoretical description to the charge transfer process.

At the end, we would like to point that the model can be developed for more realistic. Then the results in the present paper can be improved by taking into account the following points. The first one is to consider the different coupling constants between A-T and C-G pairs. The second is to consider the anharmonic oscillator of base-pairs in the case of the strong coupling. The third point, the results of path integrals can be corrected by computing the higher terms in the expansion of the velocity equation (3.13).

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